09-830/444 Buch 911554

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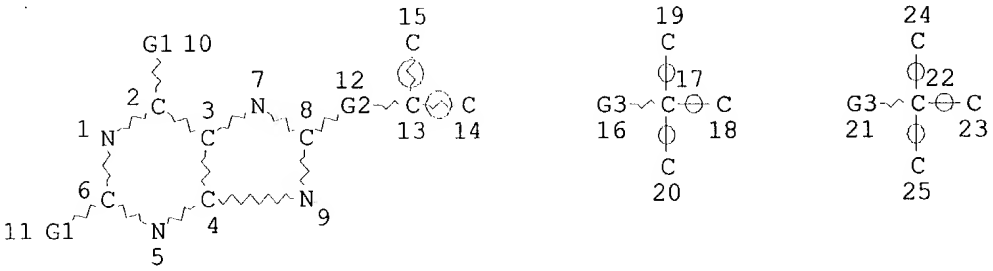


VAR G1=O/S
REP G2=(0-3) A
VAR G3=H/ME
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

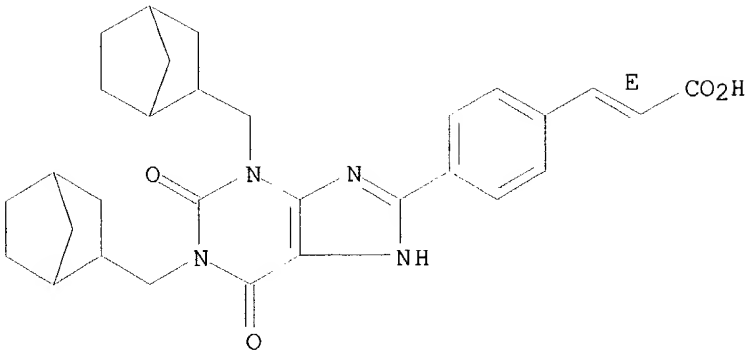
STEREO ATTRIBUTES: NONE
L5 2 SEA FILE=REGISTRY SSS FUL L3

100.0% PROCESSED 677 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.06

L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2001 ACS
RN 259254-59-6 REGISTRY
CN 2-Propenoic acid, 3-[4-[1,3-bis(bicyclo[2.2.1]hept-2-ylmethyl)-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-8-yl]phenyl]-, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H34 N4 O4
SR CA
LC STN Files: CA, CAPLUS

Double bond geometry as shown.

Prepared by M. Hale 308-4258

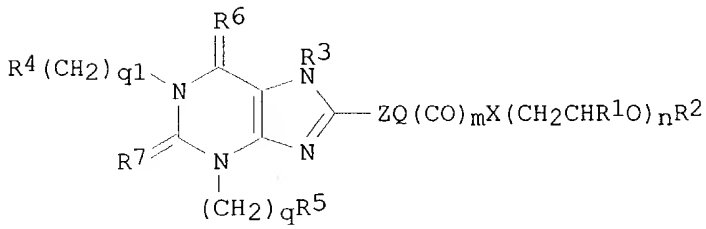


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 132:180589 Preparation of phenylxanthine derivatives as cell adhesion inhibitors.. Daluge, Susan Mary; Jurgensen, Cynthia Holder; Martin, Michael Tolar; Osterhout, Martin Howard (Glaxo Group Limited, UK).

PCT Int. Appl. WO 2000009507 A1 20000224, 101 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-EP5814 19990811. PRIORITY: GB 1998-17623 19980813.

GI



I

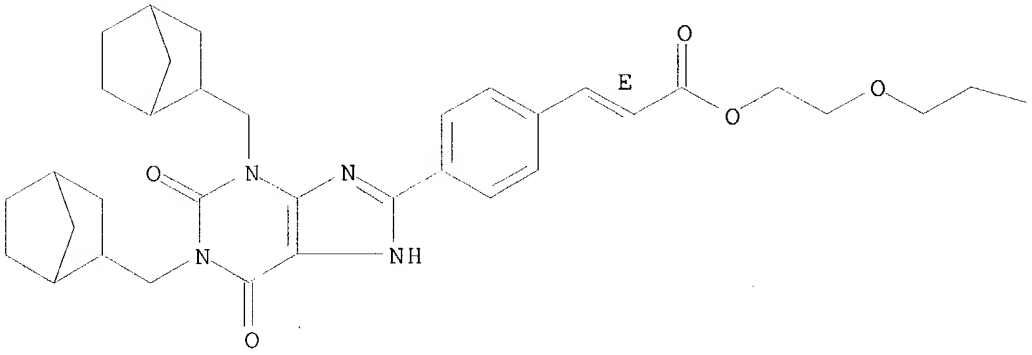
AB Title compds. [I; Z = 5-6 membered (substituted) (heteroatom-contg.) cycloalkyl, aryl; R1 = H, Me; R2 = H, alkyl, aryl, aralkyl; m = 0, 1; n = 1-50; X = O, imino, CH2O, CH2NH, etc.; Q = (CH2)p, (CH:CH)p, (C.tplbond.C)p, etc.; R3 = H, (substituted) alkyl, alkenyl, alkynyl, aminoalkyl; R4, R5 = H, cycloalkyl, alkyl, alkenyl, (substituted) aryl, heterocyclyl; R6, R7 = O, S; q, q1 = 0-10; with provisos], were prepd. Thus, (E)-4-[1,3-bis(benzyl)-1,2,3,6-tetrahydro-2,6-dioxo-9H-purin-8-yl]cinnamic acid (prepn. given) in DMF was heated to near reflux and treated with carbonyldiimidazole followed by stirring for 18 h to give

(E)-1,3-bis(benzyl)-8-[3-[2-(1H-imidazol-1-ylcarbonyl)vinyl]phenyl]-9H-purin-2,6(1H,3H)-dione. The latter was refluxed 20 h with nonaethylene glycol monomethyl ether and K2CO3 in MeCN to give 59% (E)-4-[1,3-bis(benzyl)-1,2,3,6-tetrahydro-2,6-dioxo-9H-purin-8-yl]cinnamic acid nonaethylene glycol Me ether ester. I inhibited adhesion of leukocytes to endothelial cell monolayers with IC50's of <0.1 nM to >1000 nM.

L5 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2001 ACS
RN 259254-58-5 REGISTRY
CN 2-Propenoic acid, 3-[4-[1,3-bis(bicyclo[2.2.1]hept-2-ylmethyl)-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-8-yl]phenyl]-, 3,6,9,12,15,18,21,24,27-nonaoxaoctacos-1-yl ester, (2E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C49 H72 N4 O13
SR CA
LC STN Files: CA, CAPLUS

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

PAGE 1-C

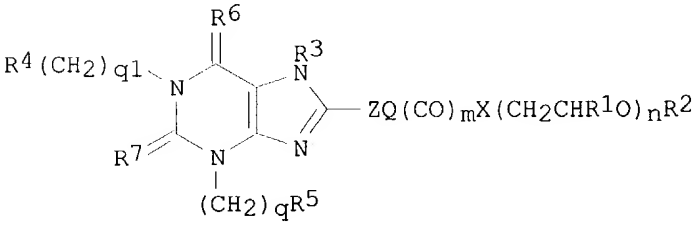
OMe

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 132:180589 Preparation of phenylxanthine derivatives as cell adhesion inhibitors.. Daluge, Susan Mary; Jurgensen, Cynthia Holder; Martin, Michael Tolar; Osterhout, Martin Howard (Glaxo Group Limited, UK).

PCT Int. Appl. WO 2000009507 A1 20000224, 101 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-EP5814 19990811. PRIORITY: GB 1998-17623 19980813.

GI



I

AB Title compds. [I; Z = 5-6 membered (substituted) (heteroatom-contg.) cycloalkyl, aryl; R1 = H, Me; R2 = H, alkyl, aryl, aralkyl; m = 0, 1; n = 1-50; X = O, imino, CH2O, CH2NH, etc.; Q = (CH2)p, (CH:CH)p, (C.tplbond.C)p, etc.; R3 = H, (substituted) alkyl, alkenyl, alkynyl, aminoalkyl; R4, R5 = H, cycloalkyl, alkyl, alkenyl, (substituted) aryl, heterocyclyl; R6, R7 = O, S; q, q1 = 0-10; with provisos], were prepd. Thus, (E)-4-[1,3-bis(benzyl)-1,2,3,6-tetrahydro-2,6-dioxo-9H-purin-8-yl]cinnamic acid (prepn. given) in DMF was heated to near reflux and treated with carbonyldiimidazole followed by stirring for 18 h to give (E)-1,3-bis(benzyl)-8-[3-[2-(1H-imidazol-1-ylcarbonyl)vinyl]phenyl]-9H-purin-2,6(1H,3H)-dione. The latter was refluxed 20 h with nonaethylene glycol monomethyl ether and K2CO3 in MeCN to give 59% (E)-4-[1,3-bis(benzyl)-1,2,3,6-tetrahydro-2,6-dioxo-9H-purin-8-yl]cinnamic acid nonaethylene glycol Me ether ester. I inhibited adhesion of leukocytes to endothelial cell monolayers with IC50's of <0.1 nM to >1000 nM.

=> fil caol;s l5

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	143.18	143.33

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

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FULL ESTIMATED COST 0.31 143.64

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